

MM 28: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials I

Time: Tuesday 14:00–14:30

Location: C 230

MM 28.1 Tue 14:00 C 230

Structural and electronic properties of one-dimensional nanothreads derived from molecular precursors under pressure — ●SAMUEL VASCONCELOS and MICHAEL ROHLFING — Institute for Solid-State Theory, University of Münster, Germany

Low-dimensional materials has been thoroughly investigated in the recent past decades. We focus mainly on one-dimensional materials, synthesized from molecular precursors. In particular, so-called nanothreads were presented in 2016 by Fitzgibbons *et. al*, derived from benzene molecules that were connected under pressure, changing their hybridization and remaining connected afterwards. Subsequently many other molecules were investigated, showing the same behaviour.

We discuss two cases, in which new properties are obtained under the same phenomenology of transformation. On the one hand, nanothreads derived from the porphyrin family presenting a metallic behaviour, which had not yet been observed in this class of materials. On the other hand, we present a new class of nanotubes with a sp^3 -connected carbon frame derived from the kekulene family, displaying a functional tubular character. Mechanical and electronic properties will be presented, as well as the basic formation mechanisms behind

such transformations.

MM 28.2 Tue 14:15 C 230

New properties from 1D materials derived from molecules under pressure — ●SAMUEL VASCONCELOS and MICHAEL ROHLFING — Universität Münster

Low-dimensional materials has been thoroughly investigated in the recent past decades. We focused mainly in the 1D materials. The precursor of a class in particular, the so-called nanothreads was presented in 2016 by Fitzgibbons *et. al*, when benzene molecules under pressure were connected, changing their hybridization and remaining connected afterwards. Subsequently many other molecules were investigated in order to obtain the same behaviour. We present two works, in which new properties were obtained under the same phenomenology of transformation. First, nanothreads derived from the porphyrin family presenting a metallic behaviour, not yet observed in this class of materials. After we present a new class of sp^3 tubes derived from the kekulene family displaying a functional tubular character. Mechanical and electronic properties will be presented, and also the mechanisms behind such transformations are also exposed in these works.